



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:53 AM UTC

PDB ID : 3C09 / pdb_00003c09
Title : Crystal structure the Fab fragment of matuzumab (Fab72000) in complex with domain III of the extracellular region of EGFR
Authors : Ferguson, K.M.; Schmiedel, J.; Knoechel, T.
Deposited on : 2008-01-18
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

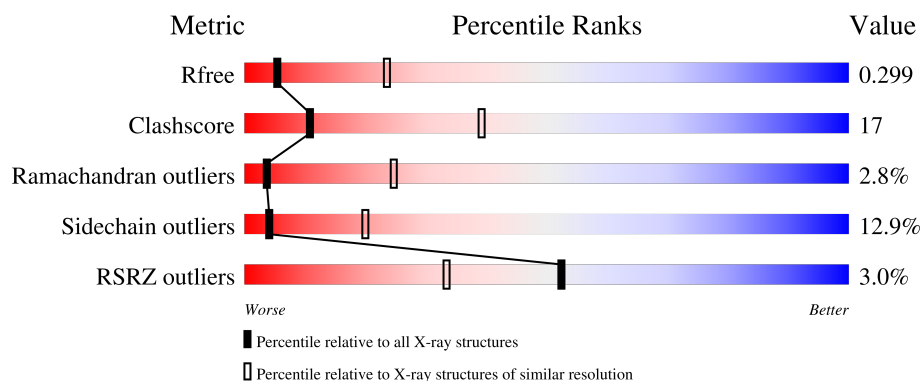
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	212	8% 52% 26% • 17%
1	L	212	68% 29% •
2	C	223	6% 58% 23% • 14%
2	H	223	65% 26% 5% •
3	A	214	57% 27% 6% 11%

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Mol	Chain	Length	Quality of chain
3	D	214	2% 59% 27% • 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Matuzumab Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1533	959	252	316	6			
1	B	175	Total	C	N	O	S	0	0	0
			1239	772	204	258	5			

- Molecule 2 is a protein called Matuzumab Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1573	996	259	311	7			
2	C	191	Total	C	N	O	S	0	0	0
			1347	846	224	270	7			

- Molecule 3 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	191	Total	C	N	O	S	0	0	0
			1371	857	237	269	8			
3	D	191	Total	C	N	O	S	0	0	0
			1296	807	226	255	8			

There are 22 discrepancies between the modelled and reference sequences:

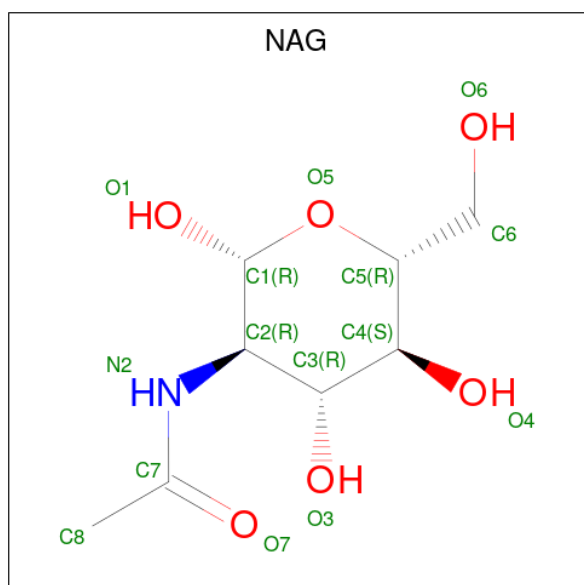
Chain	Residue	Modelled	Actual	Comment	Reference
A	307	LEU	-	expression tag	UNP P00533
A	308	GLU	-	expression tag	UNP P00533
A	309	GLU	-	expression tag	UNP P00533
A	310	LYS	-	expression tag	UNP P00533
A	311	LYS	-	expression tag	UNP P00533
A	515	HIS	-	expression tag	UNP P00533
A	516	HIS	-	expression tag	UNP P00533
A	517	HIS	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
A	518	HIS	-	expression tag	UNP P00533
A	519	HIS	-	expression tag	UNP P00533
A	520	HIS	-	expression tag	UNP P00533
D	307	LEU	-	expression tag	UNP P00533
D	308	GLU	-	expression tag	UNP P00533
D	309	GLU	-	expression tag	UNP P00533
D	310	LYS	-	expression tag	UNP P00533
D	311	LYS	-	expression tag	UNP P00533
D	515	HIS	-	expression tag	UNP P00533
D	516	HIS	-	expression tag	UNP P00533
D	517	HIS	-	expression tag	UNP P00533
D	518	HIS	-	expression tag	UNP P00533
D	519	HIS	-	expression tag	UNP P00533
D	520	HIS	-	expression tag	UNP P00533

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



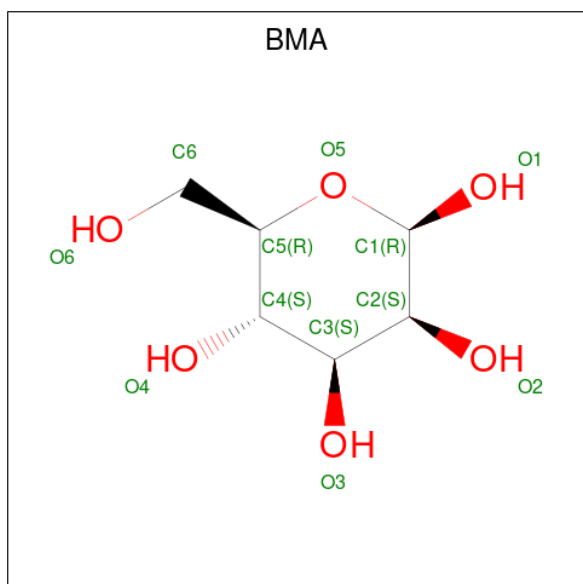
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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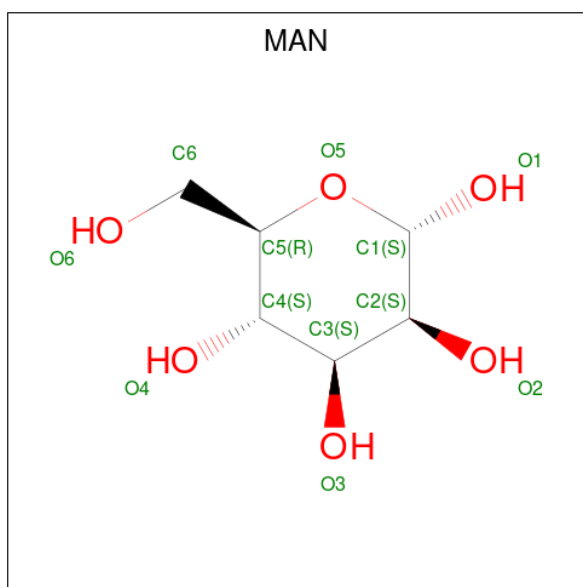
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).

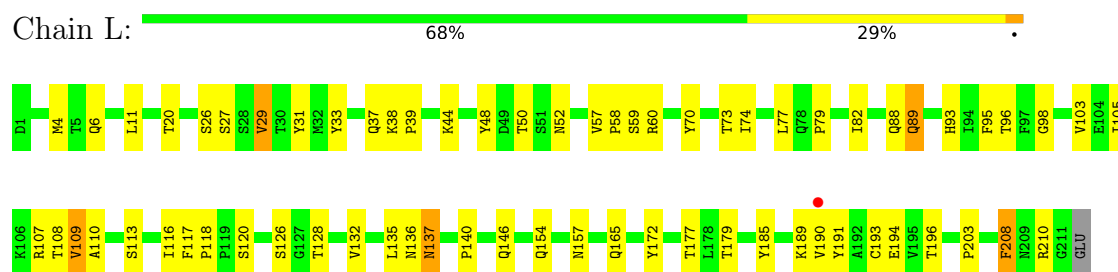


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

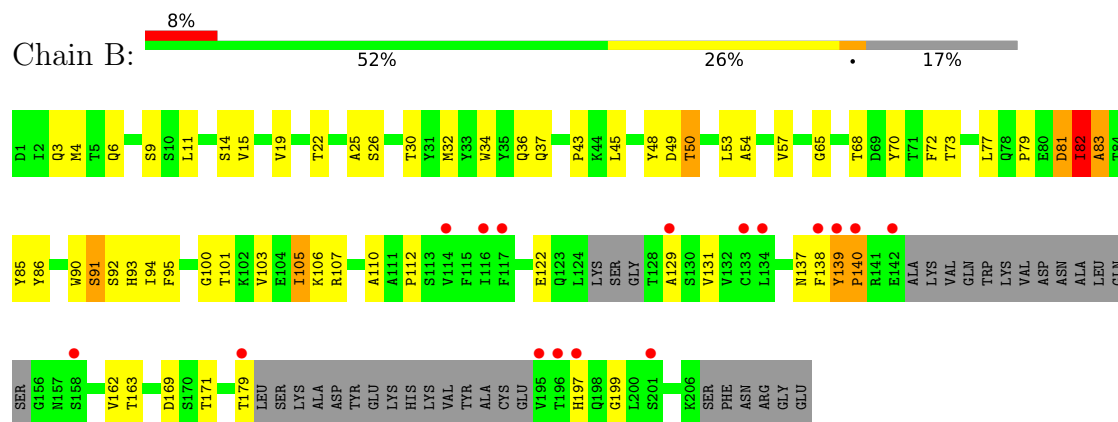
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

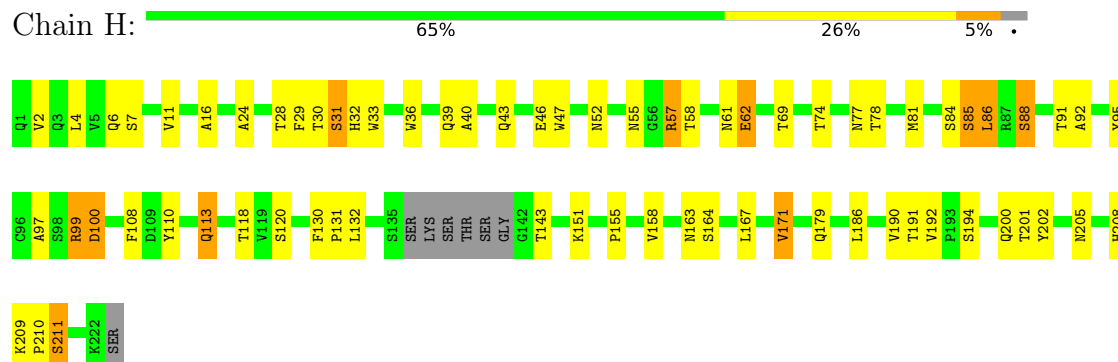
• Molecule 1: Matuzumab Fab Light chain



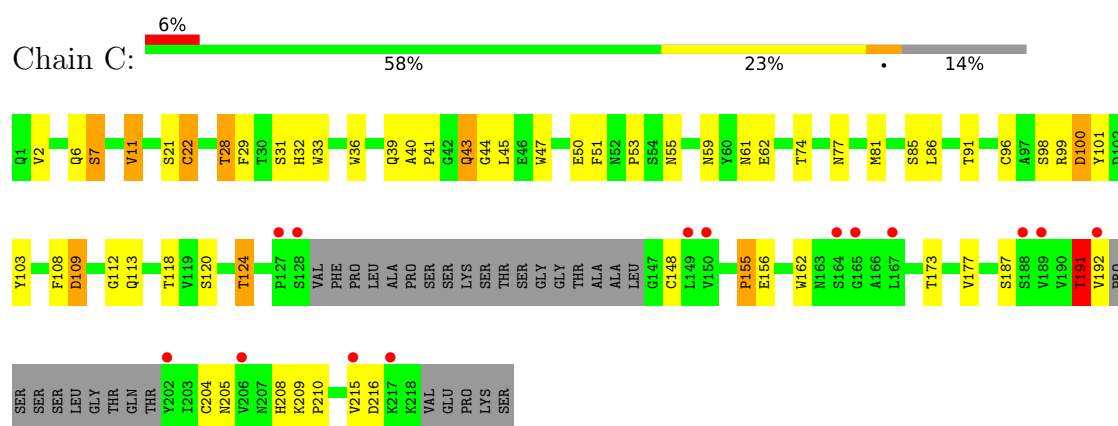
• Molecule 1: Matuzumab Fab Light chain



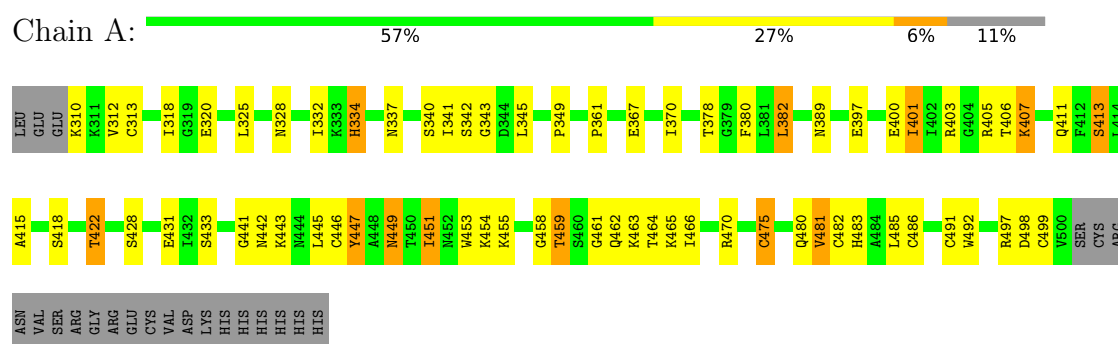
• Molecule 2: Matuzumab Fab Heavy chain



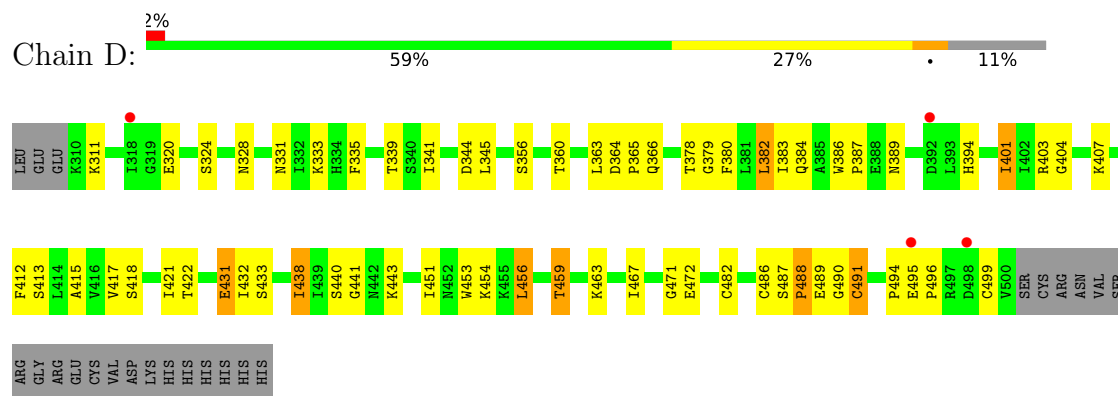
• Molecule 2: Matuzumab Fab Heavy chain



• Molecule 3: Epidermal growth factor receptor



• Molecule 3: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.07Å 205.03Å 81.58Å 90.00° 117.49° 90.00°	Depositor
Resolution (Å)	36.56 – 3.20 36.56 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.56-3.20) 99.6 (36.56-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.242 , 0.299 0.240 , 0.299	Depositor DCC
R_{free} test set	1709 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8532	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.67	0/1266	1.00	6/1732 (0.3%)
1	L	0.65	0/1570	0.93	0/2152
2	C	0.64	0/1383	0.94	1/1902 (0.1%)
2	H	0.60	0/1616	0.89	0/2223
3	A	0.62	0/1396	0.96	1/1907 (0.1%)
3	D	0.64	0/1322	1.01	6/1815 (0.3%)
All	All	0.64	0/8553	0.95	14/11731 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	360	THR	CA-C-N	8.39	125.79	119.66
3	D	360	THR	C-N-CA	8.39	125.79	119.66
1	B	83	ALA	N-CA-C	7.24	119.17	110.19
2	C	191	THR	N-CA-C	7.12	120.59	107.99
1	B	57	VAL	CA-C-N	6.96	127.00	119.90
1	B	57	VAL	C-N-CA	6.96	127.00	119.90
1	B	81	ASP	N-CA-C	-6.52	104.91	112.92
3	D	495	GLU	CA-C-N	5.84	127.14	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	495	GLU	C-N-CA	5.84	127.14	119.84
1	B	131	VAL	N-CA-C	5.73	114.99	106.85
3	D	401	ILE	N-CA-C	5.68	115.85	108.35
3	D	431	GLU	N-CA-C	5.30	117.25	108.13
3	A	361	PRO	O-C-N	5.22	123.60	121.15
1	B	82	ILE	N-CA-C	5.03	119.80	109.34

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	191	THR	Peptide
2	H	99	ARG	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1239	0	1067	59	0
1	L	1533	0	1358	49	0
2	C	1347	0	1109	37	0
2	H	1573	0	1405	40	0
3	A	1371	0	1271	49	0
3	D	1296	0	1101	37	0
4	A	84	0	78	10	0
4	D	56	0	52	5	0
5	A	11	0	10	1	0
5	D	11	0	10	0	0
6	A	11	0	10	1	0
All	All	8532	0	7471	255	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:TYR:CD2	1:B:140:PRO:HD3	1.69	1.26
1:B:139:TYR:CG	1:B:140:PRO:HD3	1.74	1.22
1:B:139:TYR:CB	1:B:140:PRO:CD	2.27	1.10
1:B:139:TYR:HB3	1:B:140:PRO:CD	1.82	1.09
1:B:139:TYR:CG	1:B:140:PRO:CD	2.41	1.03
1:L:191:TYR:HB2	1:L:208:PHE:HE1	1.21	1.01
3:A:328:ASN:HD21	4:A:3281:NAG:C1	1.74	1.00
3:D:328:ASN:HD21	4:D:3281:NAG:C1	1.74	1.00
3:A:446:CYS:HG	3:A:475:CYS:HG	1.07	0.99
1:B:139:TYR:HB3	1:B:140:PRO:HD2	1.45	0.97
1:B:139:TYR:CB	1:B:140:PRO:HD3	1.93	0.94
1:L:79:PRO:HA	1:L:105:ILE:CD1	1.98	0.93
1:L:191:TYR:HB2	1:L:208:PHE:CE1	2.06	0.90
3:D:331:ASN:HB3	4:D:3281:NAG:H61	1.55	0.89
3:A:328:ASN:ND2	4:A:3281:NAG:C1	2.35	0.89
3:A:458:GLY:H	3:A:462:GLN:HE22	1.20	0.88
2:H:32:HIS:HD2	2:H:100:ASP:OD2	1.56	0.88
3:D:382:LEU:HD11	3:D:384:GLN:HE21	1.38	0.88
1:L:118:PRO:HB3	1:L:208:PHE:CE2	2.08	0.87
1:L:146:GLN:HB3	1:L:194:GLU:HG3	1.58	0.85
1:B:30:THR:HG22	1:B:91:SER:HA	1.56	0.85
3:A:486:CYS:HG	3:A:499:CYS:HG	1.20	0.81
1:B:139:TYR:CD2	1:B:140:PRO:CD	2.61	0.81
3:A:389:ASN:HD21	4:A:3891:NAG:C1	1.94	0.81
1:B:139:TYR:HB3	1:B:140:PRO:HD3	1.55	0.81
3:D:328:ASN:ND2	4:D:3281:NAG:C1	2.42	0.81
3:A:380:PHE:HB2	3:A:413:SER:HA	1.62	0.80
3:A:482:CYS:HA	3:A:491:CYS:SG	2.22	0.79
2:H:100:ASP:OD2	3:D:454:LYS:HE3	1.84	0.76
3:A:341:ILE:HD13	3:A:345:LEU:HD21	1.68	0.75
1:B:30:THR:CG2	1:B:91:SER:HA	2.16	0.75
1:L:118:PRO:HB3	1:L:208:PHE:HE2	1.53	0.74
3:A:337:ASN:HD21	4:A:3371:NAG:C1	2.02	0.73
1:B:139:TYR:CG	1:B:140:PRO:N	2.54	0.72
3:D:378:THR:O	3:D:403:ARG:HB2	1.90	0.72
2:C:6:GLN:HE22	2:C:96:CYS:H	1.37	0.71
2:H:29:PHE:HB2	2:H:77:ASN:ND2	2.05	0.70
3:D:486:CYS:HG	3:D:499:CYS:HG	0.74	0.70
1:L:37:GLN:HE22	2:H:39:GLN:HE22	1.37	0.70
1:L:146:GLN:HB3	1:L:194:GLU:CG	2.22	0.70
1:B:11:LEU:HD21	1:B:19:VAL:HG13	1.74	0.68
1:B:36:GLN:HG3	1:B:85:TYR:CE2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:HIS:CD2	2:H:100:ASP:OD2	2.44	0.68
5:A:3283:BMA:H2	6:A:3284:MAN:C1	2.23	0.68
4:D:3281:NAG:O4	4:D:3282:NAG:C1	2.42	0.67
1:L:79:PRO:HA	1:L:105:ILE:HD12	1.75	0.67
3:A:431:GLU:OE2	3:A:433:SER:HB3	1.95	0.66
2:H:151:LYS:CE	2:H:179:GLN:HE22	2.09	0.66
1:B:45:LEU:HD21	1:B:48:TYR:HB3	1.75	0.66
2:C:33:TRP:HD1	2:C:100:ASP:OD2	1.78	0.66
3:A:458:GLY:N	3:A:462:GLN:HE22	1.93	0.65
3:A:422:THR:HG22	3:A:480:GLN:HE22	1.62	0.65
1:B:49:ASP:O	1:B:50:THR:HB	1.96	0.65
1:B:77:LEU:HD12	1:B:81:ASP:HB2	1.79	0.65
1:B:139:TYR:O	1:B:140:PRO:C	2.39	0.65
3:D:415:ALA:HA	3:D:438:ILE:HG23	1.78	0.63
4:A:3281:NAG:O4	4:A:3282:NAG:C1	2.47	0.63
2:H:6:GLN:HB2	2:H:113:GLN:HE22	1.64	0.63
1:B:77:LEU:CD1	1:B:81:ASP:HB2	2.29	0.62
3:D:341:ILE:HD13	3:D:345:LEU:HD21	1.81	0.62
2:C:99:ARG:HA	2:C:108:PHE:O	1.99	0.62
2:H:151:LYS:HE3	2:H:179:GLN:HE22	1.64	0.62
3:A:418:SER:HA	3:A:441:GLY:O	2.00	0.62
1:L:37:GLN:NE2	2:H:39:GLN:HE22	1.98	0.62
2:H:167:LEU:HD21	2:H:190:VAL:HG11	1.82	0.62
1:L:79:PRO:HA	1:L:105:ILE:HD11	1.83	0.61
3:D:432:ILE:HD12	3:D:456:LEU:HD22	1.82	0.61
1:B:34:TRP:CE2	1:B:72:PHE:HB2	2.35	0.61
3:A:332:ILE:HG13	3:A:370:ILE:HD12	1.83	0.61
2:C:40:ALA:O	2:C:43:GLN:HG3	2.00	0.61
3:A:318:ILE:HD12	3:A:342:SER:O	2.02	0.59
2:C:98:SER:O	2:C:109:ASP:HA	2.03	0.59
3:A:343:GLY:H	3:A:378:THR:HB	1.68	0.59
1:B:30:THR:HG21	1:B:90:TRP:CE3	2.38	0.59
3:A:459:THR:H	3:A:462:GLN:NE2	2.00	0.59
1:B:37:GLN:HE22	2:C:39:GLN:HE22	1.51	0.58
3:D:482:CYS:HA	3:D:491:CYS:SG	2.43	0.58
3:D:487:SER:O	3:D:489:GLU:N	2.36	0.58
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.39	0.58
3:A:451:ILE:HD12	3:A:453:TRP:CZ2	2.39	0.58
2:C:29:PHE:HB2	2:C:77:ASN:HD22	1.69	0.58
3:D:380:PHE:HB2	3:D:413:SER:HA	1.87	0.57
3:A:401:ILE:HD11	3:A:403:ARG:CZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:TRP:CD2	1:B:72:PHE:HB2	2.39	0.57
3:A:486:CYS:HA	3:A:499:CYS:SG	2.45	0.57
2:H:171:VAL:HB	2:H:190:VAL:HG22	1.86	0.56
1:B:6:GLN:NE2	1:B:101:THR:OG1	2.39	0.56
1:B:37:GLN:O	1:B:83:ALA:HB1	2.06	0.56
2:C:6:GLN:HE22	2:C:96:CYS:N	2.03	0.56
1:L:11:LEU:HD23	1:L:103:VAL:HG22	1.88	0.56
2:H:29:PHE:C	2:H:31:SER:H	2.14	0.56
2:H:208:HIS:ND1	2:H:211:SER:HB3	2.20	0.55
2:C:6:GLN:NE2	2:C:96:CYS:H	2.03	0.55
1:L:89:GLN:NE2	1:L:96:THR:HB	2.22	0.55
1:L:165:GLN:HG3	1:L:172:TYR:CZ	2.41	0.55
2:C:162:TRP:CZ3	2:C:204:CYS:HB3	2.42	0.55
3:A:459:THR:HG23	3:A:461:GLY:H	1.73	0.54
1:L:93:HIS:HA	3:D:459:THR:HG21	1.89	0.53
1:L:113:SER:HB2	1:L:136:ASN:HB3	1.90	0.53
1:L:189:LYS:HA	1:L:210:ARG:O	2.07	0.53
1:B:169:ASP:OD1	1:B:171:THR:OG1	2.23	0.53
3:D:418:SER:HA	3:D:441:GLY:O	2.09	0.53
1:B:4:MET:HE2	1:B:4:MET:HA	1.89	0.53
1:B:30:THR:CG2	1:B:90:TRP:CE3	2.91	0.53
1:L:117:PHE:CD2	2:H:132:LEU:HB3	2.43	0.53
1:B:30:THR:HG22	1:B:90:TRP:O	2.10	0.52
2:H:91:THR:HG23	2:H:118:THR:HA	1.90	0.52
1:B:65:GLY:HA3	1:B:70:TYR:CD2	2.44	0.52
2:C:32:HIS:HD2	2:C:100:ASP:CB	2.23	0.52
1:L:146:GLN:O	1:L:193:CYS:HA	2.09	0.52
2:C:28:THR:O	2:C:31:SER:HB2	2.09	0.52
3:A:459:THR:HG23	3:A:461:GLY:N	2.24	0.52
2:C:32:HIS:HD2	2:C:100:ASP:HB3	1.75	0.52
2:C:204:CYS:O	2:C:216:ASP:HB3	2.10	0.52
3:A:325:LEU:HD13	4:A:3281:NAG:H83	1.91	0.51
1:B:30:THR:HG22	1:B:91:SER:CA	2.33	0.51
1:B:82:ILE:O	1:B:103:VAL:O	2.27	0.51
2:H:11:VAL:HB	2:H:155:PRO:HG3	1.92	0.51
3:A:483:HIS:CD2	3:A:485:LEU:H	2.28	0.51
2:C:6:GLN:HE21	2:C:112:GLY:HA3	1.76	0.51
2:C:208:HIS:CE1	2:C:210:PRO:HG2	2.46	0.51
2:H:84:SER:O	2:H:85:SER:C	2.54	0.50
1:L:154:GLN:HB3	1:L:157:ASN:HD21	1.76	0.50
1:B:112:PRO:HD3	1:B:197:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:ASN:HA	2:C:216:ASP:HB3	1.93	0.50
2:C:99:ARG:HG2	2:C:109:ASP:HB2	1.94	0.50
2:H:151:LYS:HE3	2:H:179:GLN:NE2	2.27	0.50
1:B:138:PHE:O	1:B:139:TYR:O	2.30	0.49
1:L:95:PHE:HB2	2:H:47:TRP:CD2	2.47	0.49
1:B:49:ASP:O	1:B:50:THR:CB	2.60	0.49
2:H:16:ALA:O	2:H:86:LEU:HB2	2.13	0.49
1:B:138:PHE:O	1:B:138:PHE:CD1	2.65	0.49
1:B:139:TYR:HD2	1:B:140:PRO:HD3	1.60	0.49
2:C:36:TRP:CE2	2:C:81:MET:HB2	2.47	0.49
2:H:39:GLN:C	2:H:92:ALA:HB1	2.38	0.49
3:D:386:TRP:CG	3:D:387:PRO:HD2	2.48	0.49
3:A:482:CYS:SG	3:A:491:CYS:SG	3.10	0.49
3:A:380:PHE:CB	3:A:413:SER:HA	2.36	0.49
1:L:93:HIS:HD1	3:D:459:THR:HG23	1.78	0.48
1:B:106:LYS:HA	1:B:139:TYR:OH	2.13	0.48
4:A:3281:NAG:O4	4:A:3282:NAG:C2	2.61	0.48
2:C:50:GLU:HG3	2:C:59:ASN:HB2	1.96	0.48
3:D:403:ARG:HA	3:D:433:SER:HB2	1.95	0.48
1:L:89:GLN:HE22	1:L:96:THR:HB	1.79	0.48
3:A:492:TRP:H	3:A:498:ASP:HB3	1.78	0.48
1:B:197:HIS:CD2	1:B:199:GLY:H	2.31	0.48
1:L:107:ARG:NH1	1:L:110:ALA:HB2	2.29	0.47
2:H:40:ALA:O	2:H:43:GLN:HB2	2.13	0.47
2:C:91:THR:HG23	2:C:118:THR:HA	1.96	0.47
3:A:454:LYS:NZ	2:C:100:ASP:OD1	2.47	0.47
1:L:37:GLN:HE22	2:H:39:GLN:NE2	2.07	0.47
4:A:3281:NAG:C4	4:A:3282:NAG:C1	2.93	0.47
1:B:65:GLY:HA3	1:B:70:TYR:HD2	1.79	0.47
1:B:79:PRO:HA	1:B:105:ILE:HD13	1.97	0.47
2:C:47:TRP:HZ2	2:C:50:GLU:HG2	1.80	0.47
1:L:137:ASN:HA	1:L:172:TYR:O	2.15	0.47
3:A:463:LYS:HE2	2:C:101:TYR:CE1	2.50	0.47
1:L:48:TYR:O	1:L:52:ASN:HB2	2.15	0.47
1:B:32:MET:HE3	1:B:70:TYR:CD1	2.50	0.47
3:A:400:GLU:HA	3:A:428:SER:O	2.15	0.46
2:C:6:GLN:HG2	2:C:22:CYS:HB2	1.98	0.46
3:D:415:ALA:HA	3:D:438:ILE:CG2	2.46	0.46
1:L:105:ILE:O	1:L:165:GLN:NE2	2.37	0.46
3:A:367:GLU:O	3:A:370:ILE:HG13	2.16	0.46
2:C:209:LYS:N	2:C:210:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:109:VAL:HG13	1:L:140:PRO:HD3	1.98	0.46
3:A:482:CYS:HG	3:A:491:CYS:CB	2.29	0.46
2:H:209:LYS:N	2:H:210:PRO:CD	2.79	0.46
3:A:446:CYS:C	3:A:447:TYR:CD2	2.94	0.46
1:B:37:GLN:NE2	2:C:39:GLN:HE22	2.13	0.46
3:D:311:LYS:H	3:D:339:THR:HB	1.80	0.45
1:B:4:MET:HE1	1:B:25:ALA:HB2	1.99	0.45
1:B:95:PHE:HD1	2:C:47:TRP:CE2	2.34	0.45
1:L:185:TYR:CE1	1:L:191:TYR:CE2	3.05	0.45
2:H:192:VAL:HG11	2:H:202:TYR:CZ	2.52	0.45
1:L:77:LEU:HD21	1:L:105:ILE:HG12	1.99	0.45
3:D:412:PHE:CE2	3:D:438:ILE:HB	2.52	0.45
1:L:29:VAL:HB	1:L:89:GLN:HG3	1.98	0.45
2:C:11:VAL:HB	2:C:155:PRO:HG3	1.99	0.45
1:B:45:LEU:HD23	1:B:54:ALA:HB2	1.99	0.45
2:C:51:PHE:O	2:C:53:PRO:HD3	2.17	0.45
2:H:55:ASN:OD1	2:H:57:ARG:HB2	2.17	0.44
3:A:378:THR:HG23	3:A:405:ARG:HH11	1.81	0.44
3:A:459:THR:HB	1:B:93:HIS:CE1	2.52	0.44
1:B:107:ARG:HH21	1:B:110:ALA:HB2	1.82	0.44
3:D:363:LEU:O	3:D:365:PRO:HD3	2.17	0.44
1:L:33:TYR:HB2	1:L:88:GLN:HG2	1.99	0.44
2:H:61:ASN:O	2:H:62:GLU:C	2.59	0.44
1:L:60:ARG:HD2	1:L:74:ILE:HG22	2.00	0.44
1:L:120:SER:OG	2:H:130:PHE:HB3	2.17	0.44
1:L:208:PHE:CD1	1:L:208:PHE:N	2.86	0.44
2:C:7:SER:HB3	2:C:21:SER:H	1.83	0.44
2:H:164:SER:HA	2:H:205:ASN:OD1	2.18	0.44
3:A:449:ASN:HB3	2:C:103:TYR:CZ	2.53	0.44
2:H:6:GLN:N	2:H:113:GLN:OE1	2.34	0.43
3:D:344:ASP:OD1	3:D:379:GLY:HA3	2.19	0.43
1:L:6:GLN:HE21	1:L:98:GLY:HA3	1.82	0.43
1:L:29:VAL:HG13	1:L:70:TYR:OH	2.18	0.43
2:H:4:LEU:HD23	2:H:24:ALA:HA	2.01	0.43
1:B:85:TYR:O	1:B:100:GLY:HA2	2.18	0.43
3:D:364:ASP:C	3:D:366:GLN:N	2.77	0.43
1:L:57:VAL:HA	1:L:58:PRO:HD2	1.85	0.43
2:H:39:GLN:HE21	2:H:95:TYR:HE1	1.66	0.43
3:D:486:CYS:O	3:D:488:PRO:HD3	2.19	0.43
1:L:79:PRO:O	1:L:82:ILE:HD12	2.19	0.43
1:B:3:GLN:H	1:B:26:SER:HG	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:208:PHE:N	1:L:208:PHE:HD1	2.16	0.42
3:D:431:GLU:OE2	3:D:433:SER:OG	2.37	0.42
2:H:151:LYS:HE2	2:H:179:GLN:HE22	1.83	0.42
2:H:130:PHE:HA	2:H:131:PRO:HD2	1.83	0.42
1:B:129:ALA:O	1:B:179:THR:HA	2.19	0.42
3:D:394:HIS:H	3:D:394:HIS:CD2	2.37	0.42
2:H:28:THR:O	2:H:31:SER:HB2	2.18	0.42
1:B:36:GLN:HG3	1:B:85:TYR:CZ	2.55	0.42
1:B:86:TYR:HE2	2:C:44:GLY:HA2	1.84	0.42
3:D:364:ASP:C	3:D:366:GLN:H	2.26	0.42
3:A:442:ASN:HB2	3:A:445:LEU:HB3	2.01	0.42
3:A:449:ASN:C	3:A:451:ILE:H	2.28	0.42
1:L:95:PHE:HD1	2:H:47:TRP:CZ2	2.38	0.42
3:D:440:SER:HA	3:D:467:ILE:O	2.19	0.42
3:A:459:THR:H	3:A:462:GLN:HE21	1.68	0.41
1:L:4:MET:HE3	1:L:89:GLN:HB3	2.01	0.41
2:H:99:ARG:HA	2:H:108:PHE:O	2.20	0.41
3:D:364:ASP:O	3:D:366:GLN:N	2.53	0.41
1:L:107:ARG:HH12	1:L:110:ALA:HB2	1.83	0.41
2:H:33:TRP:CH2	2:H:52:ASN:HB2	2.55	0.41
3:A:380:PHE:CD2	3:A:407:LYS:HA	2.55	0.41
3:D:453:TRP:O	3:D:456:LEU:HB2	2.21	0.41
1:L:31:TYR:OH	3:D:463:LYS:HE2	2.20	0.41
3:D:380:PHE:CB	3:D:413:SER:HA	2.50	0.41
3:D:404:GLY:O	3:D:407:LYS:HE3	2.21	0.41
3:D:328:ASN:CG	4:D:3281:NAG:C1	2.93	0.41
1:L:208:PHE:HD1	1:L:208:PHE:H	1.69	0.41
3:A:341:ILE:HD12	3:A:345:LEU:HD11	2.03	0.41
3:A:481:VAL:HG12	3:A:482:CYS:H	1.86	0.41
2:C:155:PRO:HB2	2:C:156:GLU:H	1.67	0.41
3:D:451:ILE:HA	3:D:490:GLY:HA3	2.02	0.41
3:A:337:ASN:ND2	4:A:3371:NAG:H2	2.36	0.40
3:A:382:LEU:HD12	3:A:415:ALA:HB3	2.02	0.40
3:A:455:LYS:O	2:C:55:ASN:ND2	2.53	0.40
2:H:97:ALA:HA	2:H:110:TYR:O	2.21	0.40
3:A:312:VAL:HG22	3:A:340:SER:HB3	2.03	0.40
3:A:453:TRP:C	3:A:455:LYS:H	2.29	0.40
1:B:79:PRO:HA	1:B:105:ILE:CD1	2.52	0.40
3:D:333:LYS:C	3:D:335:PHE:H	2.28	0.40
3:A:337:ASN:HD21	4:A:3371:NAG:C2	2.34	0.40
1:B:37:GLN:C	1:B:83:ALA:HB1	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:CD1	1:B:105:ILE:HD12	2.52	0.40
1:L:107:ARG:HG3	1:L:108:THR:O	2.22	0.40
1:B:37:GLN:NE2	1:B:43:PRO:HD3	2.37	0.40
1:B:94:ILE:HG22	2:C:47:TRP:HZ3	1.86	0.40
2:C:61:ASN:O	2:C:62:GLU:C	2.64	0.40
1:L:38:LYS:O	1:L:39:PRO:C	2.64	0.40
1:L:117:PHE:HB2	1:L:132:VAL:HB	2.04	0.40
1:B:139:TYR:CD1	1:B:140:PRO:N	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	167/212 (79%)	145 (87%)	16 (10%)	6 (4%)	2	19
1	L	209/212 (99%)	189 (90%)	15 (7%)	5 (2%)	4	28
2	C	185/223 (83%)	159 (86%)	21 (11%)	5 (3%)	4	25
2	H	212/223 (95%)	190 (90%)	17 (8%)	5 (2%)	4	28
3	A	189/214 (88%)	153 (81%)	32 (17%)	4 (2%)	5	31
3	D	189/214 (88%)	153 (81%)	29 (15%)	7 (4%)	2	18
All	All	1151/1298 (89%)	989 (86%)	130 (11%)	32 (3%)	4	25

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	50	THR
1	B	122	GLU
1	B	139	TYR
1	B	140	PRO

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Mol	Chain	Res	Type
2	H	30	THR
2	H	85	SER
2	H	163	ASN
3	A	443	LYS
3	A	470	ARG
1	B	50	THR
1	B	82	ILE
1	B	137	ASN
2	C	85	SER
2	C	124	THR
2	C	215	VAL
3	D	472	GLU
3	D	488	PRO
2	H	88	SER
3	A	334	HIS
2	C	41	PRO
3	D	443	LYS
3	D	494	PRO
1	L	137	ASN
1	L	190	VAL
3	A	349	PRO
2	H	62	GLU
1	L	26	SER
1	L	203	PRO
3	D	471	GLY
3	D	496	PRO
3	D	421	ILE
2	C	155	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	124/188 (66%)	112 (90%)	12 (10%)	8	32
1	L	158/188 (84%)	142 (90%)	16 (10%)	7	30
2	C	122/190 (64%)	102 (84%)	20 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	159/190 (84%)	136 (86%)	23 (14%)	3	16
3	A	142/188 (76%)	120 (84%)	22 (16%)	2	14
3	D	118/188 (63%)	105 (89%)	13 (11%)	6	26
All	All	823/1132 (73%)	717 (87%)	106 (13%)	4	20

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	THR
1	L	27	SER
1	L	29	VAL
1	L	44	LYS
1	L	59	SER
1	L	73	THR
1	L	89	GLN
1	L	109	VAL
1	L	116	ILE
1	L	126	SER
1	L	128	THR
1	L	135	LEU
1	L	177	THR
1	L	179	THR
1	L	196	THR
1	L	208	PHE
2	H	2	VAL
2	H	7	SER
2	H	31	SER
2	H	46	GLU
2	H	57	ARG
2	H	58	THR
2	H	69	THR
2	H	74	THR
2	H	78	THR
2	H	86	LEU
2	H	88	SER
2	H	100	ASP
2	H	113	GLN
2	H	120	SER
2	H	143	THR
2	H	158	VAL
2	H	171	VAL

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Mol	Chain	Res	Type
2	H	186	LEU
2	H	191	THR
2	H	194	SER
2	H	200	GLN
2	H	201	THR
2	H	211	SER
3	A	310	LYS
3	A	313	CYS
3	A	320	GLU
3	A	334	HIS
3	A	382	LEU
3	A	397	GLU
3	A	401	ILE
3	A	406	THR
3	A	407	LYS
3	A	411	GLN
3	A	413	SER
3	A	422	THR
3	A	447	TYR
3	A	449	ASN
3	A	451	ILE
3	A	459	THR
3	A	464	THR
3	A	465	LYS
3	A	466	ILE
3	A	475	CYS
3	A	481	VAL
3	A	497	ARG
1	B	9	SER
1	B	14	SER
1	B	15	VAL
1	B	22	THR
1	B	53	LEU
1	B	68	THR
1	B	73	THR
1	B	91	SER
1	B	92	SER
1	B	105	ILE
1	B	162	VAL
1	B	163	THR
2	C	2	VAL
2	C	7	SER

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Mol	Chain	Res	Type
2	C	11	VAL
2	C	22	CYS
2	C	28	THR
2	C	43	GLN
2	C	45	LEU
2	C	74	THR
2	C	86	LEU
2	C	100	ASP
2	C	109	ASP
2	C	113	GLN
2	C	120	SER
2	C	124	THR
2	C	148	CYS
2	C	173	THR
2	C	177	VAL
2	C	187	SER
2	C	191	THR
2	C	192	VAL
3	D	320	GLU
3	D	324	SER
3	D	356	SER
3	D	382	LEU
3	D	383	ILE
3	D	389	ASN
3	D	401	ILE
3	D	417	VAL
3	D	422	THR
3	D	438	ILE
3	D	456	LEU
3	D	459	THR
3	D	491	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	89	GLN
1	L	157	ASN
1	L	188	HIS
1	L	197	HIS
2	H	32	HIS
2	H	39	GLN

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Mol	Chain	Res	Type
2	H	59	ASN
2	H	163	ASN
2	H	172	HIS
2	H	179	GLN
2	H	200	GLN
3	A	328	ASN
3	A	337	ASN
3	A	389	ASN
3	A	462	GLN
3	A	480	GLN
3	A	483	HIS
1	B	37	GLN
1	B	197	HIS
2	C	6	GLN
2	C	32	HIS
2	C	43	GLN
2	C	77	ASN
2	C	212	ASN
3	D	384	GLN
3	D	394	HIS
3	D	398	ASN
3	D	480	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	3282	-	14,14,15	0.72	0	17,19,21	1.70	3 (17%)
4	NAG	A	3371	-	14,14,15	0.54	0	17,19,21	1.78	4 (23%)
4	NAG	A	4202	-	14,14,15	0.54	0	17,19,21	1.04	0
5	BMA	D	3283	-	11,11,12	0.54	0	15,15,17	1.41	1 (6%)
5	BMA	A	3283	-	11,11,12	0.44	0	15,15,17	0.70	0
4	NAG	A	3891	-	14,14,15	0.59	0	17,19,21	1.12	2 (11%)
4	NAG	D	3282	-	14,14,15	0.66	0	17,19,21	1.59	2 (11%)
4	NAG	D	3371	-	14,14,15	0.52	0	17,19,21	1.37	2 (11%)
4	NAG	D	3891	-	14,14,15	0.56	0	17,19,21	0.65	0
6	MAN	A	3284	-	11,11,12	0.47	0	15,15,17	1.32	2 (13%)
4	NAG	A	3281	-	14,14,15	0.84	1 (7%)	17,19,21	1.85	3 (17%)
4	NAG	A	4201	-	14,14,15	0.61	0	17,19,21	1.52	3 (17%)
4	NAG	D	3281	-	14,14,15	0.66	0	17,19,21	1.54	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	3282	-	-	1/6/23/26	0/1/1/1
4	NAG	A	3371	-	-	2/6/23/26	0/1/1/1
4	NAG	A	4202	-	-	2/6/23/26	0/1/1/1
5	BMA	D	3283	-	-	0/2/19/22	0/1/1/1
5	BMA	A	3283	-	-	1/2/19/22	0/1/1/1
4	NAG	A	3891	-	-	3/6/23/26	0/1/1/1
4	NAG	D	3282	-	-	4/6/23/26	0/1/1/1
4	NAG	D	3371	-	-	3/6/23/26	0/1/1/1
4	NAG	D	3891	-	-	2/6/23/26	0/1/1/1
6	MAN	A	3284	-	-	1/2/19/22	0/1/1/1
4	NAG	A	3281	-	-	2/6/23/26	0/1/1/1
4	NAG	A	4201	-	-	4/6/23/26	0/1/1/1
4	NAG	D	3281	-	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3281	NAG	O5-C1	-2.16	1.40	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3281	NAG	O5-C1-C2	-5.41	102.92	111.29
4	D	3371	NAG	C1-O5-C5	4.53	118.26	112.19
4	A	4201	NAG	C3-C4-C5	4.33	118.08	110.23
4	A	3371	NAG	C3-C4-C5	4.28	117.99	110.23
4	A	3282	NAG	O5-C1-C2	-4.16	104.85	111.29
5	D	3283	BMA	C3-C4-C5	4.11	117.68	110.23
6	A	3284	MAN	C1-O5-C5	3.99	117.53	112.19
4	A	3282	NAG	C4-C3-C2	-3.61	105.73	111.02
4	A	3281	NAG	C3-C4-C5	3.56	116.68	110.23
4	D	3282	NAG	O5-C1-C2	-3.51	105.85	111.29
4	D	3282	NAG	C3-C4-C5	3.45	116.49	110.23
4	D	3281	NAG	C3-C4-C5	3.23	116.09	110.23
4	A	3371	NAG	O5-C1-C2	-3.13	106.44	111.29
4	A	3281	NAG	C2-N2-C7	-3.08	118.77	122.90
4	A	4201	NAG	O5-C1-C2	-3.03	106.61	111.29
4	A	3371	NAG	C1-O5-C5	2.79	115.93	112.19
4	D	3371	NAG	O5-C1-C2	2.67	115.42	111.29
4	A	3891	NAG	C3-C4-C5	2.56	114.88	110.23
4	D	3281	NAG	O5-C1-C2	-2.52	107.39	111.29
4	A	3891	NAG	O5-C1-C2	-2.51	107.40	111.29
4	D	3281	NAG	O3-C3-C4	-2.40	104.71	110.38
4	A	3371	NAG	O5-C5-C4	2.39	116.64	110.83
6	A	3284	MAN	O5-C1-C2	2.34	116.37	110.79
4	A	3282	NAG	C2-N2-C7	-2.17	119.99	122.90
4	A	4201	NAG	C4-C3-C2	2.00	113.95	111.02

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3891	NAG	C8-C7-N2-C2
4	A	3891	NAG	O7-C7-N2-C2
4	D	3371	NAG	C8-C7-N2-C2
4	D	3371	NAG	O7-C7-N2-C2
4	D	3282	NAG	C8-C7-N2-C2
4	D	3282	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	D	3891	NAG	O7-C7-N2-C2
4	A	3281	NAG	O5-C5-C6-O6
4	D	3891	NAG	C8-C7-N2-C2
4	A	4201	NAG	O5-C5-C6-O6
4	A	3371	NAG	C4-C5-C6-O6
4	D	3282	NAG	O5-C5-C6-O6
4	A	3281	NAG	C4-C5-C6-O6
4	A	4201	NAG	C4-C5-C6-O6
4	A	4202	NAG	O5-C5-C6-O6
4	A	3371	NAG	O5-C5-C6-O6
4	D	3281	NAG	O5-C5-C6-O6
4	A	4201	NAG	C8-C7-N2-C2
6	A	3284	MAN	O5-C5-C6-O6
4	D	3282	NAG	C4-C5-C6-O6
4	A	4201	NAG	O7-C7-N2-C2
4	D	3371	NAG	C4-C5-C6-O6
4	A	3891	NAG	O5-C5-C6-O6
4	A	3282	NAG	O5-C5-C6-O6
4	A	4202	NAG	C4-C5-C6-O6
5	A	3283	BMA	C4-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3282	NAG	3	0
4	A	3371	NAG	3	0
5	A	3283	BMA	1	0
4	A	3891	NAG	1	0
4	D	3282	NAG	1	0
6	A	3284	MAN	1	0
4	A	3281	NAG	6	0
4	D	3281	NAG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	175/212 (82%)	0.40	16 (9%) 15 9	27, 40, 96, 100	0
1	L	211/212 (99%)	0.10	1 (0%) 87 76	25, 42, 73, 83	0
2	C	191/223 (85%)	0.46	14 (7%) 21 13	34, 51, 81, 83	0
2	H	216/223 (96%)	0.09	0 100 100	31, 50, 63, 69	0
3	A	191/214 (89%)	0.09	0 100 100	34, 47, 76, 81	0
3	D	191/214 (89%)	0.33	4 (2%) 63 43	44, 53, 89, 94	0
All	All	1175/1298 (90%)	0.24	35 (2%) 52 33	25, 49, 82, 100	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	VAL	4.1
1	B	196	THR	3.8
2	C	127	PRO	3.7
2	C	128	SER	3.6
1	B	140	PRO	3.4
1	B	134	LEU	3.3
2	C	149	LEU	3.3
2	C	189	VAL	3.3
2	C	164	SER	3.2
2	C	188	SER	3.1
2	C	150	VAL	3.1
2	C	206	VAL	3.0
1	B	129	ALA	3.0
1	B	179	THR	3.0
2	C	165	GLY	2.9
1	B	114	VAL	2.8
3	D	498	ASP	2.8
1	B	201	SER	2.8
2	C	192	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	139	TYR	2.5
3	D	318	ILE	2.5
1	B	117	PHE	2.5
1	B	142	GLU	2.4
1	B	116	ILE	2.3
1	B	158	SER	2.3
1	L	190	VAL	2.3
2	C	215	VAL	2.2
3	D	392	ASP	2.2
2	C	217	LYS	2.2
1	B	133	CYS	2.2
1	B	197	HIS	2.1
2	C	202	TYR	2.1
3	D	495	GLU	2.1
2	C	167	LEU	2.0
1	B	138	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BMA	A	3283	11/12	0.65	0.18	108,108,108,109	0
4	NAG	D	3371	14/15	0.68	0.16	104,106,106,107	0
4	NAG	A	4202	14/15	0.68	0.14	102,103,103,103	0
5	BMA	D	3283	11/12	0.70	0.17	111,112,112,112	0
4	NAG	A	3891	14/15	0.73	0.13	99,100,100,100	0
4	NAG	D	3891	14/15	0.74	0.11	96,97,98,98	0
4	NAG	A	3371	14/15	0.76	0.15	82,85,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	A	3284	11/12	0.76	0.12	91,94,95,95	0
4	NAG	A	4201	14/15	0.79	0.13	76,78,78,78	0
4	NAG	D	3282	14/15	0.93	0.10	67,70,73,74	0
4	NAG	A	3282	14/15	0.94	0.10	52,54,55,57	0
4	NAG	A	3281	14/15	0.96	0.09	31,35,42,42	0
4	NAG	D	3281	14/15	0.96	0.08	33,37,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.